Journal of Computational and Applied Mathematics 231 (2009) 948–963

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Quadrature formulas on the unit circle with prescribed nodes and maximal domain of validity

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ARTICLE INFO

Article history:
Received 3 September 2008
Received in revised form 6 May 2009

MSC:
42C05
41A55

Keywords:
Laurent polynomials
Gauss–Lobatto quadrature
Interpolatory quadrature
Error estimates

ABSTRACT

In this paper we investigate the Szegő–Radau and Szegő–Lobatto quadrature formulas on the unit circle. These are $(n+m)$-point formulas for which m nodes are fixed in advance, with $m = 1$ and $m = 2$ respectively, and which have a maximal domain of validity in the space of Laurent polynomials. This means that the free parameters (free nodes and positive weights) are chosen such that the quadrature formula is exact for all powers z^j, $-p \le j \le p$, with $p = p(n, m)$ as large as possible.

1. Introduction

In this paper we consider quadrature formulas of the form

$$\int_{-\pi}^{\pi} f(\mathrm{e}^{\mathrm{i}\theta})\mathrm{d}\mu(\theta) \approx \sum_{j=1}^{m} A_j f(x_j) + \sum_{k=1}^{n} \lambda_k f(z_k).$$

We assume that μ is some finite positive Borel measure supported on $[-\pi, \pi]$. The integrands will all be defined on the unit circle, that is on $\mathbb{T} := \{z \in \mathbb{C} : |z| = 1\}$. Thus setting $z = \mathrm{e}^{\mathrm{i}\theta}$, it makes sense to write $\int f \mathrm{d}\mu$. In the rest of this paper we shall always assume that z stands for $\mathrm{e}^{\mathrm{i}\theta}$ when z appears under an integral sign.

The quadrature formula is a linear combination of function values in x_j and z_k. The m nodes $x_j \in \mathbb{T}$ will be fixed in advance while the n remaining values, also in $\mathbb{T}$, can be chosen freely. Once the nodes are chosen, it is clear that by integrating a Laurent polynomial $L \in \Lambda_{p,q} := \operatorname{span}\{z^p, z^{p+1}, \ldots, z^q\}$ with $q - p = n + m$, interpolating f in the $n + m$ nodes, will give corresponding weights A_j and λ_k that make the quadrature formula exact for all $f \in \Lambda_{p,q}$. However, since the choice of the nodes $z_k \in \mathbb{T}$ is still free, we can make use of this freedom to make the quadrature formula exact in a larger space $\Lambda_{r,s} \supset \Lambda_{p,q}$. The objective is to make the dimension of the space $\Lambda_{r,s}$ as large as possible. We then have a maximal domain of validity. It is usual to choose the domain of validity in a balanced way, i.e., $r = -s$.

For solving this problem, orthogonal polynomials play a central role. So we introduce an inner product for functions defined on the unit circle with respect to the measure μ as follows:

$$\langle f, g\rangle_\mu := \int_{-\pi}^{\pi} \overline{f(\mathrm{e}^{\mathrm{i}\theta})} g(\mathrm{e}^{\mathrm{i}\theta})\mathrm{d}\mu(\theta). \tag{1.1}$$

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doi:10.1016/j.cam.2009.05.019

We also use the notation $f_*(z) := \overline{f(1/\overline{z})}$ for the para-hermitian conjugate. Note that for $z \in \mathbb{T}$, the para-hermitian conjugate is just the usual complex conjugate: $f_*(z) = \overline{f(z)}$.

Now consider the sequence of polynomials $\{1, z, z^2, \ldots\}$ and orthogonalize them with respect to this inner product, giving a sequence of Szegő polynomials $\{\rho_0, \rho_1, \rho_2, \ldots\}$. For $n > 0$, the polynomial ρ_n is defined (up to a constant multiple) by

$$\left\langle z^k, \rho_n \right\rangle_\mu = 0, \quad k = 0, \ldots, n-1, \qquad \left\langle z^n, \rho_n \right\rangle_\mu \neq 0.$$

For any polynomial $p_n \in \Pi_n := \Lambda_{0,n}$, we also introduce the adjoint defined as $p_n^*(z) := z^n p_{n*}(z) \in \Pi_n$.

Unlike the formulas for Gauss quadrature, zeros of orthogonal polynomials are not suitable as nodes in a quadrature formula because they are all in the open unit disk $\mathbb{D} := \{z \in \mathbb{C} : |z| < 1\}$, and neither are the zeros of ρ_n^*, because these are all in the exterior of the closed unit disk $\mathbb{E} := \{z \in \mathbb{C} : |z| > 1\}$.

This problem is solved by considering para-orthogonal polynomials. Their orthogonality properties will be given in the next section. Para-orthogonal polynomial do have simple zeros that are all on $\mathbb{T}$. Hence they can be used as nodes in a quadrature formula.

If, in our general quadrature problem we set $m = 0$, i.e., there are no fixed nodes, and if we choose the nodes z_k as the zeros of the para-orthogonal polynomials, we obtain the Szegő quadrature formulas having a maximal domain of validity $\Lambda_{-(n-1),n-1}$, (see [1]). These are the analogues on the unit circle of the Gauss quadrature formulas on an interval of the real line. In this case, the weights λ_k are guaranteed to be positive, which is important for numerical stability and convergence of the quadratures.

Our main interest however will be in considering the cases $m = 1$ and $m = 2$, which will be called the Szegő–Radau and the Szegő–Lobatto cases, in analogy with the Gaussian situation where one or two nodes are fixed, usually in one or both endpoints of the interval. Clearly there are no endpoints on a circle and the prefixed nodes are permitted to be any point of $\mathbb{T}$. The Szegő–Radau and Szegő–Lobatto quadrature formulas have been recently studied by Jagels and Reichel [2]. We shall of course come to the same conclusions but use a different approach.

The outline of the paper is as follows. In Section 2 we introduce some preliminaries and give a general result on the quadrature formulas with maximal domain of validity and m prefixed nodes with m arbitrary. The Szegő–Radau formulas with one fixed node are considered in Section 3. We shall show that these formulas with fixed node x_1 for $\mathrm{d}\mu$ are actually ordinary Szegő formulas for $\mathrm{d}\tilde{\mu}(\theta) = |e^{i\theta} - x_1|^2 \mathrm{d}\mu(\theta)$. Section 4 considers the Szegő–Lobatto formulas. Finally in Section 5 we give some simple error estimates and prove convergence while in Section 6 we include some numerical examples.

2. Preliminary results

Let us first recall the setting for usual Szegő quadrature formulas. For the positive Borel measure on $[-\pi, \pi]$ we define its trigonometric moments as

$$\mu_k := \int_{-\pi}^{\pi} e^{-ik\theta} \mathrm{d}\mu(\theta), \quad k = 0, \pm 1, \pm 2, \ldots. \tag{2.1}$$

and an inner product $\langle f, g \rangle_\mu$ as in (1.1). The integral

$$I_\mu(f) := \int_{-\pi}^{\pi} f(e^{i\theta}) \mathrm{d}\mu(\theta) \tag{2.2}$$

can be approximated by a quadrature formula of the form

$$I_n(f) := \sum_{j=1}^{n} \lambda_i f(z_i). \tag{2.3}$$

The distinct nodes $\{z_i\}_{i=1}^n \subset \mathbb{T}$ and the positive weights $\{\lambda_i\}_{i=1}^n$, are defined by imposing that $I_\mu(L) = I_n(L)$ for all $L \in \Lambda_{-p(n),p(n)}$ with $p(n)$ as large as possible. It is well known that $p(n)$ cannot exceed $n-1$ and the "optimal" situation $p(n) = n-1$, corresponds to the Szegő quadrature formulas, as we already mentioned in the previous section. The following result is well known (see [1]) and implies that the maximal domain of validity is reached by a quadrature formula if and only if it is a Szegő quadrature.

Theorem 2.1. *Let $I_n(f) = \sum_{i=1}^n \lambda_i f(z_i)$ have distinct nodes $z_i \in \mathbb{T}$, $i = 1, \ldots, n$ and define the nodal polynomial $Q_n(x) := \prod_{j=1}^n (z - z_j)$. Then $I_n(f) = I_\mu(f)$, $\forall f \in \Lambda_{-(n-1),n-1}$ if and only if*

(1) *$I_n(f)$ is exact in $\Lambda_{-p,q}$ with p and q nonnegative integers such that $p + q = n - 1$*
(2) *$Q_n(z)$ is invariant, i.e., $Q_n^*(z) = KQ_n(z)$, $K \neq 0$, for all $z \in \mathbb{C}$ and satisfies*
   (a) $\left\langle Q_n, z^j \right\rangle_\mu = 0$, $1 \leq j \leq n-1$
   (b) $\langle Q_n, 1 \rangle_\mu \langle Q_n, z^n \rangle_\mu \neq 0$.

A polynomial of degree n satisfying the above orthogonality condition is called *para-orthogonal* (see [1]) with respect to the measure μ.

The quadrature formulas as given in the theorem were introduced by Jones et al. [1] (see also [3]). They are "optimal" in the sense that there cannot exist an n-point quadrature rule with nodes on $\mathbb{T}$ that is exact in $\Lambda_{-n,n}$, but neither can such a formula be exact in $\Lambda_{-n,n-1}$ nor in $\Lambda_{-(n-1),n}$.

Theorem 2.1, also implies that the only way to produce an n-point quadrature formula with nodes on $\mathbb{T}$ and having a maximal domain of validity is by taking as nodes the zeros of a polynomial of degree n which is both para-orthogonal and invariant. Such polynomials have the following fundamental properties [1].

Theorem 2.2. *Let $B_n(z)$ be a polynomial of degree n, para-orthogonal and invariant, then*

(1)
$$B_n(z) = B_n(z, \tau) = c_n[\rho_n(z) + \tau\rho_n^*(z)], \quad c_n \neq 0, |\tau| = 1 \tag{2.4}$$
(2)
$$B_n(z) = B_n(z, \tilde{\tau}) = \tilde{c}_n[z\rho_{n-1}(z) + \tilde{\tau}\rho_{n-1}^*(z)], \quad \tilde{c}_n \neq 0, |\tilde{\tau}| = 1 \tag{2.5}$$
(3) *$B_n(z)$ has exactly n distinct zeros on $\mathbb{T}$.*

From Theorems 2.1 and 2.2, we see that the existence of Szegő quadrature formulas is guaranteed. However, unlike the Gaussian formulas, Szegő formulas depend on a parameter τ, a fact that will be exploited in the next section. Furthermore, the weights λ_i are positive, so that convergence in the class of bounded functions integrable with respect to μ can be assured [4].

Quadrature formulas on the unit circle and related topics (Szegő polynomials, trigonometric moment problem,...) have become a productive research area. However, these quadratures have not been studied as exhaustively as the Gaussian formulas. The problem we consider is to prefix some nodes and to find optimal locations for the remaining ones so as to obtain a maximal domain of validity. Its precise statement is as follows.

Problem 2.3. Given m distinct nodes $x_1, \ldots, x_m \in \mathbb{T}$ and given $n \in \mathbb{N}$, find n distinct nodes z_k on $\mathbb{T} \setminus \{x_1, \ldots, x_m\}$ and positive weights $A_1, \ldots, A_m, \lambda_1, \ldots, \lambda_n$, such that

$$I_{n+m}(f) := \sum_{j=1}^{m} A_j f(x_j) + \sum_{k=1}^{n} \lambda_k f(z_k) \tag{2.6}$$

satisfies

$$I_{n+m}(R) = I_\mu(R), \quad \forall R \in \Lambda_{-p,p}$$

with $p = p(n, m)$ a nonnegative integer as large as possible.

Since we have $2n+m$ unknowns and $\dim(\Lambda_{-p,p}) = 2p+1$, we will first impose that $2p+1 \geq 2n+m$, i.e., $p \geq n+E[\frac{m-1}{2}]$ where $E[x]$ denotes the largest integer $\leq x$.

On the other hand, as we are handling $n+m$ nodes, the maximum domain of validity that might be reached is $\Lambda_{-(n+m-1),n+m-1}$ so that we have for $p = p(n, m)$ the following restriction

$$n + E\left[\frac{m-1}{2}\right] \leq p \leq n+m-1. \tag{2.7}$$

Now, we can analyse the following particular cases to which we will restrict ourselves, namely

(1) $m = 0$. In this case no node is given in advance so that (2.7) becomes $n-1 \leq p \leq n-1$, i.e., $p = n-1$. Here the maximum domain of validity is $\Lambda_{-(n-1),n-1}$ and the resulting quadrature formulas are the Szegő formulas.
(2) $m = 1$. Now, only the node x_1 is prescribed on $\mathbb{T}$ and (2.7) gives rise to $p = n$. That is, if an appropriate quadrature formula
$$I_{n+1}(f) = A_1 f(x_1) + \sum_{j=1}^{n} \lambda_j f(z_j)$$
exists, then it should be exact in $\Lambda_{-n,n}$. This can be considered as a Radau formula on $\mathbb{T}$ and as we will see later, its study simply reduces to conveniently fix the parameter $\tau \in \mathbb{T}$ which characterizes the Szegő quadrature formula.
(3) $m = 2$. Now two nodes x_1 and x_2 are fixed in advance and from (2.7) we have $n \leq p \leq n+1$. Thus we have two cases that are to be analysed.
   (a) $p = n$. This yields a domain of validity $\Lambda_{-n,n}$ for a quadrature formula with $n+2$ nodes. If it exists in the sense that distinct nodes can be found on $\mathbb{T}$ so that the formula is exact in $\Lambda_{-n,n}$, then it cannot be a Szegő formula anymore, which implies that it cannot be assured that the weights are positive.
   (b) $p = n+1$. This gives rise to a quadrature formula with $n+2$ nodes and domain of validity $\Lambda_{-(n+1),n+1}$. Thus, if it exists, it is actually an $(n+2)$-point Szegő formula for $I_\mu(f)$.

   Both situations can be considered as the analogue on $\mathbb{T}$ of the well-known Gauss–Lobatto formulas for the real line. For this reason, the terminology Szegő–Lobatto formulas was adopted in [2] were they have been recently introduced.

As a preliminary result, let us give a characterization for quadrature formulas with prescribed nodes on $\mathbb{T}$.

Theorem 2.4. *Consider m distinct nodes $x_1, \ldots, x_m$ on $\mathbb{T}$ and define*

$$I_{n+m}(f) := \sum_{j=1}^{m} A_j f(x_j) + \sum_{k=1}^{n} \lambda_k f(z_k)$$

with distinct nodes $\{z_k\}_{k=1}^{n} \subset \mathbb{T} \setminus \{x_j\}_{j=1}^{m}$. Set

$$Q_{n+m}(z) := \prod_{j=1}^{m}(z-x_j)\prod_{k=1}^{n}(z-z_k).$$

Furthermore assume that $n \geq 1$ if m is odd and $n \geq 2$ if m is even. Then $I_{n+m}(f)$ is exact in $\Lambda_{-p,p}$ with $p = p(n, m)$ a nonnegative integer satisfying (2.7) if and only if

(1) *$I_{n+m}(f)$ is exact in $\Lambda_{-r,s}$, r and s being integers such that $0 \leq r, s \leq p$ and $r + s = n + m - 1$.*

(2)

$$\left\langle Q_{n+m}(z), z^j\right\rangle_\mu = 0, \quad n+m-p \leq j \leq p. \tag{2.8}$$

Furthermore, when $\Lambda_{-p,p}$ is a maximal domain of validity, i.e., $I_{n+m}(f)$ cannot be exact either in $\Lambda_{-p,p+1}$ or in $\Lambda_{-(p+1),p}$, then it also holds that $\left\langle Q_{n+m}(z), z^{n+m-p-1}\right\rangle_\mu \left\langle Q_{n+m}(z), z^{p+1}\right\rangle_\mu \neq 0$.

Note that (2.7) together with (2.8) implies that $n + m - p \leq p$ or $n + m \leq 2p = 2n + m - 1$ if m is odd and $n + m \leq 2p = 2n + m - 2$ if m is even. Thus $n \geq 1$ if m is odd and $n \geq 2$ if m is even, which makes (2.8) meaningful.

Proof. "$\Rightarrow$" (1) This trivially follows since $\Lambda_{-r,s} \subset \Lambda_{-p,p}$.

(2) Take $n + m - p \leq j \leq p$. Then

$$\left\langle Q_{n+m}(z), z^j\right\rangle_\mu = \int_{-\pi}^{\pi} \frac{Q_{n+m}(z)}{z^j} \mathrm{d}\mu(\theta), \quad z = \mathrm{e}^{\mathrm{i}\theta}.$$

Now $z^{-j}Q_{n+m}(z) \in \Lambda_{-j,n+m-j}$ and from the above condition it follows that $\Lambda_{-j,n+m-j} \subset \Lambda_{-p,p}$. Hence

$$\left\langle Q_{n+m}(z), z^j\right\rangle_\mu = I_\mu\left(z^{-j}Q_{n+m}(z)\right) = I_{n+m}\left(z^{-j}Q_{n+m}(z)\right) = 0.$$

"$\Leftarrow$" Take r and s as above and consider $\Lambda_{-r,s}$ with dimension $r + s + 1 = n + m$. Since we have $m + n$ distinct nodes on $\mathbb{T}$ and $n + m$ weights that we shall denote by $A_1, \ldots, A_m, \lambda_1, \ldots, \lambda_n$, these can be uniquely determined such that

$$I_{n+m}(f) = \sum_{j=1}^{m} A_j f(x_j) + \sum_{k=1}^{n} \lambda_k f(z_k) = I_\mu(f), \quad \forall f \in \Lambda_{-r,s}.$$

To see this, take into account that $\{z^j\}_{j=1}^{s}$ is a Chebyshev system on $\mathbb{T}$. Take now $f \in \Lambda_{-p,p}$ and consider $L \in \Lambda_{-r,s}$ such that $f(x_j) = L(x_j)$, $j = 1, \ldots, m$ and $f(z_k) = L(z_k)$, $k = 1, \ldots, n$. Then, $R(z) = f(z) - L(z) \in \Lambda_{-p,p}$ vanishes for $z \in \{x_1, \ldots, x_m, z_1, \ldots, z_n\}$.

Thus we can write

$$R(z) = Q_{n+m}(z) \cdot z^{-p}P(z), \quad P \in \Pi_{2p-(n+m)}.$$

Note that $z^{-p}P(z) \in \operatorname{span}\{z^{-j} : m + n - p \leq j \leq p\}$. So $I_\mu(f) = I_\mu(L + R) = I_\mu(L) + I_\mu(R) = I_n(L) + I_\mu(R) = I_n(f) + I_\mu(R)$. It remains to show that $I_\mu(R) = 0$, and that follows from the orthogonality conditions in (2.8).

In a similar way it can be shown that if $\left\langle Q_{n+m}(z), z^{n+m-p-1}\right\rangle_\mu = 0$ or $\left\langle Q_{n+m}(z), z^{p+1}\right\rangle_\mu = 0$, then the quadrature formula would have a domain of validity $\Lambda_{-(p+1),p}$ or $\Lambda_{-p,p+1}$ respectively, which would contradict the fact that the domain of validity $\Lambda_{-p,p}$ is maximal. □

Remark 2.5. Note that for $m = 0$, Theorem 2.1 is recovered as a special case of Theorem 2.4.

3. Szegő–Radau formulas

Assume that x_1 is a fixed point on $\mathbb{T}$. In this section we shall be concerned with quadrature formulas of the form

$$I_{n+1}(f) := A_1 f(x_1) + \sum_{k=1}^{n} \lambda_k f(z_k) \tag{3.1}$$

where the nodes $\{z_k\}_{k=1}^{n}$ and the weights $\{A_1, \lambda_1, \ldots, \lambda_n\}$ are to be determined so that

$$I_{n+1}(f) = I_\mu(f), \quad \forall f \in \Lambda_{-p(n),p(n)}$$

with $p(n)$ as large as possible. Furthermore, we also require that the weights in (3.1) are positive. As seen in Section 2, $p(n) = n$ and the nodal polynomial $Q_{n+1}(z) = (z - x_1)\prod_{k=1}^{n}(z - z_k)$ from Theorem 2.4 should satisfy the orthogonality conditions

$$\left\langle Q_{n+1}(z), z^j \right\rangle_\mu = 0, \quad 1 \le j \le n, \tag{3.2}$$

i.e., Q_{n+1} is a polynomial of degree $n+1$ para-orthogonal with respect to μ. Therefore

$$Q_{n+1}(z) = c_{n+1}[\rho_{n+1}(z) + \tau \rho^*_{n+1}(z)], \quad \tau \in \mathbb{T}, c_{n+1} \neq 0.$$

It is now a simple matter to see that the parameters $\tau \in \mathbb{T}$ can be chosen so that x_1 is a zero of the corresponding para-orthogonal polynomial of degree $n+1$ for this parameter. Hence the resulting $(n+1)$-point quadrature formula with x_1 as a node will be exact in $\Lambda_{-n,n}$ and the weights are positive.

Indeed, from Theorems 2.1 and 2.2, one knows that $\forall \tau \in \mathbb{T}$, the zeros of $B_{n+1}(z) = B_{n+1}(z, \tau) = \rho_{n+1}(z) + \tau \rho^*_{n+1}(z)$ produce an $(n+1)$-point quadrature formula with positive weights and exact in $\Lambda_{-n,n}$. Now $B_{n+1}(x_1) = 0$ implies

$$\tau = -\frac{\rho_{n+1}(x_1)}{\rho^*_{n+1}(x_1)} \tag{3.3}$$

(observe that this is well defined since $\rho^*_{n+1}(z) \neq 0$ for $z \in \mathbb{T}$) and

$$|\tau| = \left| \frac{\rho_{n+1}(x_1)}{\rho^*_{n+1}(x_1)} \right| = \left| \frac{\rho_{n+1}(x_1)}{x_1^{n+1} \overline{\rho_{n+1}(x_1)}} \right| = 1.$$

Thus from Theorems 2.1 and 2.2 and using the classical formulas for the weights of Szegő quadrature formulas [4], we can prove that the following holds true.

Proposition 3.1. *Let $x_1 \in \mathbb{T}$ be fixed and take τ as given by (3.3) and set $B_{n+1}(z) := \rho_{n+1}(z) + \tau \rho^*_{n+1}(z)$. Then one has*

(1) $B_{n+1}(z) = c_{n+1}(z - x_1) \prod_{k=1}^n (z - z_k)$, $c_{n+1} \neq 0$, $x_1 \neq z_k \in \mathbb{T}$, $k = 1, \ldots, n$.

(2) *Define* ($z = e^{i\theta}$)

$$\lambda_k := \frac{1}{|B'_{n+1}(z_k)|^2} \int_{-\pi}^{\pi} \left| \frac{B_{n+1}(z)}{z - z_k} \right|^2 d\mu(\theta) > 0, \quad k = 1, \ldots, n$$

and

$$A_1 := \frac{1}{|B'_{n+1}(x_1)|^2} \int_{-\pi}^{\pi} \left| \frac{B_{n+1}(z)}{z - x_1} \right|^2 d\mu(\theta) > 0,$$

then

$$I_{n+1}(f) = A_1 f(x_1) + \sum_{k=1}^n \lambda_k f(z_k) = I_\mu(f), \quad \forall f \in \Lambda_{-n,n}. \tag{3.4}$$

Remark 3.2. According to [2], $I_{n+1}(f)$ given by (3.4) will be called the Szegő–Radau formula for the measure μ with fixed node x_1.

Remark 3.3. When assuming that the trigonometric moments μ_n are real (for example when μ is symmetric, i.e., $d\mu(\theta) = d\mu(-\theta)$) then the Szegő polynomials have real coefficients so that for $x_1 = \pm 1$, it follows from (3.3) that $\tau = -1/x_1^{n+1}$, yielding $\tau = -1$ when $x_1 = 1$ and $\tau = (-1)^n$ when $x_1 = -1$. In these cases, one sees that the parameter τ is independent of the corresponding sequence of Szegő polynomials.

Now set $B_{n+1}(z) := (z - x_1) \prod_{k=1}^n (z - z_k) = (z - x_1) Q_n(z)$ with $Q_n(z) \in \Pi_n$ and define a new measure $d\tilde{\mu}(\theta) := |z - x_1|^2 d\mu(\theta)$, $(z = e^{i\theta})$. Let $\{\tilde{\rho}_n(z)\}$ be its sequence of monic Szegő polynomials, then we have the following property.

Proposition 3.4. *Let $Q_n(z)$ be as given above, then there exists a $\tilde{\tau} \in \mathbb{T}$ and $\tilde{c}_n \neq 0$ such that*

$$Q_n(z) = \tilde{c}_n [\tilde{\rho}_n(z) + \tilde{\tau} \tilde{\rho}^*_n(z)]. \tag{3.5}$$

Proof. It is sufficient to check that Q_n is invariant and para-orthogonal with respect to $\tilde{\mu}$. Invariance trivially follows since the zeros of Q_n are on $\mathbb{T}$. On the other hand, for k such that $1 \le k \le n-1$, and $z = e^{i\theta}$

$$\begin{aligned}
\left\langle Q_n, z^k \right\rangle_{\tilde{\mu}} &= \int_{-\pi}^{\pi} Q_n(z) z^{-k} |z - x_1|^2 d\mu(\theta) \\
&= \int_{-\pi}^{\pi} Q_n(z)(z - x_1)(\bar{z} - \bar{x}_1) z^{-k} d\mu(\theta) \\
&= \int_{-\pi}^{\pi} B_{n+1}(z)(z^{-1} - x_1^{-1}) z^{-k} d\mu(\theta) \\
&= \left\langle B_{n+1}, z^{k+1} \right\rangle_\mu - \bar{x}_1 \left\langle B_{n+1}, z^k \right\rangle_\mu = 0
\end{aligned}$$

since $\langle B_{n+1}, z^j\rangle_\mu = 0$ for $1 \le j \le n$. Furthermore

$$\begin{aligned}\langle Q_n, 1\rangle_{\tilde\mu} &= \int_{-\pi}^{\pi} Q_n(z)(z-x_1)(\bar z - \bar x_1)\mathrm{d}\mu(\theta)\\ &= \int_{-\pi}^{\pi} B_{n+1}(z)(\bar z - \bar x_1)\mathrm{d}\mu(\theta)\\ &= \langle B_{n+1}, z\rangle_\mu - \bar x_1 \langle B_{n+1}, 1\rangle = -\bar x_1 \langle B_{n+1}, 1\rangle_\mu \ne 0.\end{aligned}$$

Similarly $\langle Q_n, z^n\rangle_{\tilde\mu} \ne 0$.

As for the computation of the parameter $\tilde\tau$, we can write without loss of generality that

$$B_{n+1}(z) = \rho_{n+1}(z) + \tau\rho^*_{n+1}(z)$$

with τ given by (3.3) so that $B_{n+1}(z) = (z - x_1)Q_n(z)$ where $Q_n(z)$ is given by

$$Q_n(z) = \tilde c_n[\tilde\rho_n(z) + \tilde\tau\tilde\rho^*_n(z)], \quad \tilde c_n \ne 0, \tilde\tau \in \mathbb{T}.$$

By comparing the leading coefficient in $\rho_{n+1}(z) + \tau\rho^*_{n+1}(z) = \tilde c_n[(z - x_1)(\tilde\rho_n(z) + \tilde\tau\tilde\rho^*_n(z))]$ it follows that $1 + \tau\bar\delta_{n+1} = \tilde c_n(1 + \tilde\tau\bar{\tilde\delta}_n)$ where $\{\delta_n\}_0^\infty$ and $\{\tilde\delta_n\}_0^\infty$ represent the corresponding sequence of Schur parameters for $\mathrm{d}\mu$ and $\mathrm{d}\tilde\mu$ respectively.

On the other hand, a comparison of the constant terms gives:

$$\delta_{n+1} + \tau = -x_1\tilde c_n(\tilde\delta_n + \tilde\tau)$$

yielding

$$\frac{1 + \tau\bar\delta_{n+1}}{1 + \tilde\tau\bar{\tilde\delta}_n} = -\frac{\tau + \delta_{n+1}}{x_1(\tilde\delta_n + \tilde\tau)}.$$

Setting $A := 1 + \tau\bar\delta_{n+1}$ and $B := (\tau + \delta_{n+1})/x_1$, we have

$$\tilde\tau = -\frac{\tilde\delta_n + C}{1 + C\bar{\tilde\delta}_n} \quad \text{where } C := \frac{B}{A} = \frac{1}{x_1}\frac{\tau + \delta_{n+1}}{1 + \tau\bar\delta_{n+1}}. \tag{3.6}$$

Observe that $|C| = 1$ implies that $\tilde\tau$ has modulus 1, as was to be expected. □

Let us now see what happens with the weights $A_1, \lambda_1, \dots, \lambda_n$ of the $(n+1)$-point Szegő–Radau formula.

On the one hand, given the zeros $z_1, \dots, z_n$ of Q_n, we can construct the n-point Szegő formula for $\mathrm{d}\tilde\mu$, with $\tilde\tau$ given by (3.6), namely

$$\tilde I_n(f) := \sum_{k=1}^{n} \tilde\lambda_k f(z_k) = I_{\tilde\mu}(f) := \int_{-\pi}^{\pi} f(\mathrm{e}^{\mathrm{i}\theta})\mathrm{d}\tilde\mu(\theta), \quad \forall f \in \Lambda_{-(n-1),n-1}. \tag{3.7}$$

On the other hand, we have also an $(n+1)$-point Szegő–Radau formula for $I_\mu(f)$ exact in $\Lambda_{-n,n}$ given by

$$I_{n+1}(f) := A_1 f(x_1) + \sum_{k=1}^{n} \lambda_k f(z_k) = I_\mu(f), \quad \forall f \in \Lambda_{-n,n}. \tag{3.8}$$

Let us next reveal the relation between the weights $\{\lambda_k\}_{k=1}^n$ and $\{\tilde\lambda_k\}_{k=1}^n$. Therefore, recall that $B_{n+1}(z) = (z - x_1)Q_n(z)$ and consequently

$$B'_{n+1}(z_j) = (z_j - x_1)Q'_n(z_j), \quad \text{and} \quad B'_{n+1}(x_1) = Q_n(x_1), \tag{3.9}$$

Furthermore, it is also known (see e.g. [4]) that for $j = 1, \dots, n$ $(z = \mathrm{e}^{\mathrm{i}\theta})$

$$\lambda_j = \frac{1}{B'_{n+1}(z_j)}\int_{-\pi}^{\pi}\frac{B_{n+1}(z)}{z - x_1}\mathrm{d}\mu(\theta). \tag{3.10}$$

$$\tilde\lambda_j = \frac{1}{Q'_n(z_j)}\int_{-\pi}^{\pi}\frac{Q_n(z)}{z - z_j}\mathrm{d}\tilde\mu(\theta). \tag{3.11}$$

Therefore

$$\begin{aligned}\tilde\lambda_j &= \frac{1}{Q'_n(z_j)}\int_{-\pi}^{\pi}\frac{Q_n(z)}{z - z_j}(z - x_1)(\bar z - \bar x_1)\mathrm{d}\mu(\theta)\\ &= \frac{1}{Q'_n(z_j)}\int_{-\pi}^{\pi}\frac{B_{n+1}(z)}{z - z_j}(\bar z - \bar x_1)\mathrm{d}\mu(\theta)\\ &= -\frac{\bar x_1}{Q'_n(z_j)}\int_{-\pi}^{\pi}\frac{B_{n+1}(z)}{z - z_j}\mathrm{d}\mu(\theta) + \frac{1}{Q'_n(z_j)}\int_{-\pi}^{\pi}\frac{B_{n+1}(z)}{z(z - z_j)}\mathrm{d}\mu(\theta).\end{aligned}$$

Since

$$\frac{1}{z(z-z_j)} = \frac{1}{z_j}\left[\frac{1}{z-z_j} - \frac{1}{z}\right],$$

it follows that

$$\tilde{\lambda}_j = -\frac{\overline{x}_1(z_j - x_1)}{B'_{n+1}(z_j)}\int_{-\pi}^{\pi}\frac{B_{n+1}(z)}{z-z_j}\mathrm{d}\mu(\theta) + \frac{z_j - x_1}{z_j B'_{n+1}(z_j)}\int_{-\pi}^{\pi}\frac{B_{n+1}(z)}{z-z_j}\mathrm{d}\mu(\theta) - \frac{1}{z_j Q'_n(z_j)}\left\langle B_{n+1}, z\right\rangle_{\mu}.$$

Since $\left\langle B_{n+1}, z\right\rangle_{\mu} = 0$, we deduce $\tilde{\lambda}_j = (1 - z_j/x_1)\lambda_j + (z_j - x_1)/z_j\lambda_j = [2 - (z_j\overline{x}_1 + x_1\overline{z}_j)]\lambda_j$, yielding

$$\lambda_j = \frac{\tilde{\lambda}_j}{2(1 - \mathrm{Re}(z_j\overline{x}_1))}, \quad j = 1, \dots, n. \tag{3.12}$$

(Observe that $\mathrm{Re}(z_j\overline{x}_1) \neq 1$, otherwise $|z_j\overline{x}_1| = 1$ and $\mathrm{Re}(z_j\overline{x}_1) = 1$ would imply $z_j = x_1$ which is excluded.) Finally, for the weight A_1, we have

$$A_1 = \mu_0 - (\lambda_1 + \lambda_2 + \cdots + \lambda_n).$$

In short, the computation of the $(n+1)$-point Szegő–Radau formula eventually reduces to the computation of the n-point Szegő formula for the new measure $\mathrm{d}\tilde{\mu}(\theta) := |z - x_1|^2\mathrm{d}\mu(\theta)$, where the trigonometric moments $\tilde{\mu}_k$ can be easily expressed in terms of the trigonometric moments μ_k of the original measure $\mathrm{d}\mu$ by means of

$$\tilde{\mu}_k = 2\mu_k - \overline{x}_1\mu_{k-1} - x_1\mu_{k+1}, \quad k = 0, \pm 1, \pm 2, \dots. \tag{3.13}$$

Remark 3.5. As for an efficient computation of the $(n+1)$th Szegő–Radau formula, once x_1 has been fixed on $\mathbb{T}$, one starts from the Schur parameters $\delta_n = \rho_n(0)$, $n = 0, 1, \dots$ ($\delta_0 = 1$, $|\delta_n| = 1$). By means of the recurrence relations (Levinson algorithm), one computes the parameter

$$\tau = -\frac{\rho_{n+1}(x_1)}{x_1^{n+1}\overline{\rho_{n+1}(x_1)}}.$$

($\tau = -x_1\rho_n(x_1)/\rho_n^*(x_1)$ as follows from Theorem 2.2 (2).) Then the computation of the $(n+1)$-point Szegő–Radau formula can be found by computing the eigenvalues and eigenvectors of Hessenberg matrices [2,5] or five-diagonal matrices as recently shown in [6], see also [7,8]. In both cases we are dealing with matrices of order $n+1$.

However, from Proposition 3.4, and formula (3.12), computations involving matrices of order n suffice. For this approach, it is essential to express the Schur parameters $\tilde{\delta}_n$ for $\mathrm{d}\tilde{\mu}(\theta) = |z - x_1|^2\mathrm{d}\mu(\theta)$ in terms of the Schur parameters δ_n for $\mathrm{d}\mu(\theta)$. Therefore we refer to [9], where it is shown that for $|\beta| = 1$, one can express the monic orthogonal polynomial $\tilde{\rho}_n(z)$ with respect to $\mathrm{d}\tilde{\mu}$, in terms of the monic orthogonal polynomial $\rho_{n+1}(z)$ with respect to $\mathrm{d}\mu$ as follows:

$$(z-\beta)^2\tilde{\rho}_n(z) = \frac{1}{\begin{vmatrix}\rho_{n+1}(\beta) & \rho^*_{n+1}(\beta)\\ \rho'_{n+1}(\beta) & \rho^{*\prime}_{n+1}(\beta)\end{vmatrix}}\begin{vmatrix}(z-\beta)\rho_{n+1}(z) & \rho_{n+1}(z) & \rho^*_{n+1}(z)\\ 0 & \rho_{n+1}(\beta) & \rho^*_{n+1}(\beta)\\ \rho_{n+1}(\beta) & \rho'_{n+1}(\beta) & \rho^{*\prime}_{n+1}(\beta)\end{vmatrix}.$$

So, if we take $\beta = x_1$ and $z = 0$, and setting

$$k(x_1) := \begin{vmatrix}\rho_{n+1}(x_1) & \rho^*_{n+1}(x_1)\\ \rho'_{n+1}(x_1) & \rho^{*\prime}_{n+1}(x_1)\end{vmatrix}, \tag{3.14}$$

we get by expansion along the first column:

$$\begin{aligned} x_1^2\tilde{\delta}_n &= \frac{1}{k(x_1)}\Big(-x_1\delta_{n+1}k(x_1) + \rho_{n+1}(x_1)\big(\delta_{n+1}\rho^*_{n+1}(x_1) - \rho_{n+1}(x_1)\big)\Big)\\ &= -x_1\delta_{n+1} + \frac{\rho_{n+1}(x_1)}{k(x_1)}\big(\delta_{n+1}\rho^*_{n+1}(x_1) - \rho_{n+1}(x_1)\big). \end{aligned} \tag{3.15}$$

To simplify this expression, we introduce the function $\tau_{n+1}(z) = -\rho_{n+1}(z)/\rho^*_{n+1}(z)$. Then

$$\tau'_{n+1}(z) = \frac{\rho_{n+1}(z)\rho^{*\prime}_{n+1}(z) - \rho'_{n+1}(z)\rho^*_{n+1}(z)}{\big(\rho^*_{n+1}(z)\big)^2},$$

and thus

$$k(x_1) = \tau'_{n+1}(x_1)\big(\rho^*_{n+1}(x_1)\big)^2.$$

Note that from the Christoffel–Darboux relation [7] for monic Szegő polynomials

$$k_n(z,w) := \sum_{k=0}^{n} \frac{\rho_k(z)\overline{\rho_k(w)}}{\|\rho_k\|^2} = \frac{\rho_{n+1}^*(z)\overline{\rho_{n+1}^*(w)} - \rho_{n+1}(z)\overline{\rho_{n+1}(w)}}{\|\rho_{n+1}\|^2(1-z\overline{w})}$$

it follows that by taking the superstar conjugate with respect to w we also have for any $w \neq 0$

$$w^n \sum_{k=0}^{n} \frac{\rho_k(z)\rho_{k*}(w)}{\|\rho_k\|^2} = \frac{\rho_{n+1}^*(z)\rho_{n+1}(w) - \rho_{n+1}(z)\rho_{n+1}^*(w)}{\|\rho_{n+1}\|^2(w-z)}.$$

If in this formula we first set $z = x_1 \in \mathbb{T}$ and then let $w \to x_1$, we obtain that it equals

$$k(x_1) = \tau_{n+1}'(x_1)(\rho_{n+1}^*(x_1))^2 = x_1^n\|\rho_{n+1}\|^2 \sum_{k=0}^{n} \frac{|\rho_k(x_1)|^2}{\|\rho_k\|^2} = \|\rho_{n+1}\|^2 x_1^n k_n(x_1,x_1).$$

Hence with this notation we get from our previous expression (3.15)

$$\begin{aligned} x_1^2\tilde{\delta}_n &= -x_1\delta_{n+1} + \frac{\rho_{n+1}(x_1)}{k(x_1)}\left(\delta_{n+1}\rho_{n+1}^*(x_1) - \rho_{n+1}(x_1)\right) \\ &= -x_1\delta_{n+1} + \frac{\rho_{n+1}(x_1)}{\|\rho_{n+1}\|^2 x_1^n k_n(x_1,x_1)}(0-x_1)\|\rho_{n+1}\|^2 x_1^n \sum_{k=0}^{n} \frac{\rho_k(0)\overline{\rho_k(x_1)}}{\|\rho_k\|^2} \\ &= -x_1\delta_{n+1} - x_1\rho_{n+1}(x_1)\frac{k_n(0,x_1)}{k_n(x_1,x_1)}. \end{aligned}$$

Thus if we know all the δ_k, we can generate the ρ_k and hence also the reproducing kernels $k_n(z,w)$, so that $\tilde{\delta}_n$ is computable in principle. In some simple cases, this may lead to explicit expressions like the following example illustrates.

Example 3.6. Consider the Lebesgue measure $d\mu(\theta) = d\theta$, then the Szegő polynomials are simply $\rho_n(z) = z^n$, and the Schur parameters are $\delta_0 = 1$ and $\delta_k = 0$ for $k = 1, 2, \ldots$. Now consider the measure $d\tilde{\mu}(\theta) = |e^{i\theta} - x_1|^2 d\theta$, then $k_n(0,x_1) = 1$ and $k_n(x_1,x_1) = \sum_{k=0}^{n} |x_1|^{2k} = n+1$ and hence $x_1^2\tilde{\delta}_n = -x_1^{n+2}/(n+1)$, and this eventually leads to $\tilde{\delta}_n = x_1^n/(n+1)$. Note that this also follows directly from formulas (3.14)–(3.15).

4. Szegő–Lobatto formulas

Throughout this section we assume that x_1 and x_2 on $\mathbb{T}$ are given such that $x_1 \neq x_2$. We shall be concerned with the problem of finding $z_1, \ldots, z_n$ also on $\mathbb{T}$ so that $z_j \neq z_k$ if $j \neq k$ and $z_k \neq x_j$, $k = 1, \ldots, n$, $j = 1, 2$ along with positive weights $A_1, A_2, \lambda_1, \ldots, \lambda_n$ so that

$$I_{n+2}(f) := A_1 f(x_1) + A_2 f(x_2) + \sum_{k=1}^{n} \lambda_k f(z_k) = I_\mu(f), \quad \forall f \in \Lambda_{-p(n),p(n)} \tag{4.1}$$

with $p(n)$ as high as possible. From Section 2, it follows that $n \le p(n) \le n+1$. When $p(n) = n+1$, then $I_{n+2}(f)$ would be exact in $\Lambda_{-(n+1),n+1}$ so that we should be dealing with an $(n+2)$-point Szegő quadrature formula, provided that it exists so that all the requirements (distinct nodes on $\mathbb{T}$ and positive weights) would be satisfied. On the other hand, when $p(n) = n$, and if a solution to the above problem exists, then it holds that $I_{n+2}(f) = I_\mu(f)$, $\forall f \in \Lambda_{-n,n}$.

Observe that we have $2n+2$ parameters available and $\dim(\Lambda_{-n,n}) = 2n+1$, so that we could also try with a domain of the form $\Lambda_{-n,(n+1)}$ or $\Lambda_{-(n+1),n}$ who both have a dimension $2n+2$. However, because of the requirement that the weights have to be positive in (4.1), exactness in $\Lambda_{-n,(n+1)}$ or $\Lambda_{-(n+1),n}$ automatically implies exactness in $\Lambda_{-(n+1),n+1}$. For this reason, we will initially try to find a quadrature formula of the form (4.1) which is exact at least in $\Lambda_{-n,n}$ and whose coefficients are positive. In this case, it will be said that $I_{n+2}(f)$, if it exists, represents a Szegő–Lobatto formula for $I_\mu(f)$ with prescribed nodes x_1 and x_2 on $\mathbb{T}$.

First, from Theorem 2.4, we have the the following corollary.

Corollary 4.1. *Let x_1 and x_2 be distinct nodes on $\mathbb{T}$ and set*

$$I_{n+2}(f) := A_1 f(x_1) + A_2 f(x_2) + \sum_{k=1}^{n} \lambda_k f(z_k) \approx I_\mu(f)$$

where $\{z_j\}_{j=1}^n$ are distinct nodes in $\mathbb{T} \setminus \{x_1, x_2\}$. Set

$$Q_{n+2}(z) := (z-x_1)(z-x_2)\prod_{j=1}^{n}(z-z_j).$$

Then, $I_{n+2}(f)$ is exact in $\Lambda_{-n,n}$ if and only if

(1) *$I_{n+2}(f)$ is exact in $\Lambda_{-p,q}$, p and q being integers such that $0 \le p, q \le n$ and $p+q = n+1$.*
(2)

$$\left\langle Q_{n+2}(z), z^j \right\rangle_\mu = 0, \quad 2 \le j \le n. \tag{4.2}$$

Remark 4.2. Setting $Q_{n+2}(z) = (z-x_1)(z-x_2)Q_n(z)$, with $Q_n(z) = \prod_{j=1}^n (z-z_j)$, then it easily follows that (4.2) is equivalent to the fact that $Q_n(z)$ is para-orthogonal with respect to the complex measures ($z = \mathrm{e}^{\mathrm{i}\theta}$)

$$\mathrm{d}\tilde{\mu}(\theta) = (1 - x_1\bar{z})(z - x_2)\mathrm{d}\mu(\theta) \quad \text{or} \quad \mathrm{d}\tilde{\mu}(\theta) = (1 - x_2\bar{z})(z - x_1)\mathrm{d}\mu(\theta).$$

Thus setting $x_1 = \mathrm{e}^{\mathrm{i}\alpha}$ when $x_2 = \bar{x}_1$, it results in $\mathrm{d}\tilde{\mu}(\theta) = 2(\cos\theta - \cos\alpha)\mathrm{d}\mu(\theta)$. So in the case of a pair of fixed complex conjugate nodes, we have para-orthogonality with respect to a real measure with changing sign, so that nothing can be assured initially about the zeros of $Q_n(z)$.

By Corollary 4.1 and from an algebraic point of view, our problem reduces to studying the existence and characterization of a polynomial $Q_{n+2}(z)$ of degree $n+2$ such that

$$\begin{aligned} &Q_{n+2}(x_1) = 0 = Q_{n+2}(x_2) \\ &\left\langle Q_{n+2}, z^j \right\rangle_\mu = 0, \quad 2 \le j \le n. \end{aligned} \tag{4.3}$$

Thus we see that (4.3) is a homogeneous linear system with $n+1$ equations and $n+3$ unknowns (the coefficients of $Q_{n+2}(z) = \sum_{j=0}^{n+2} c_j z^j$). Hence (4.3) always admits a nontrivial solution. But, furthermore, the solution should meet with the following requirements

(1) $c_{n+2} \neq 0$, i.e., Q_{n+2} has exact degree $n+2$
(2) Its zeros $\{x_1, x_2, z_1, \ldots, z_n\}$ should all be distinct and lie on $\mathbb{T}$.
(3) The weights in $I_{n+2}(f)$ given by (4.1) must be positive.

But, since the solution in (4.1) depends on two free parameters, one could conveniently choose them in order to satisfy the above requirements. For our purposes, we will proceed in an alternative way. Taking into account that the zeros of the para-orthogonal polynomials are distinct and on $\mathbb{T}$, our main aim is to impose para-orthogonality on Q_{n+2}. From (4.2) we see that two conditions are lacking:

$$\langle Q_{n+2}, z \rangle_\mu = 0 \quad \text{and} \quad \left\langle Q_{n+2}, z^{n+1} \right\rangle_\mu = 0. \tag{4.4}$$

Furthermore, the orthogonality relations (4.2) depend essentially on the trigonometric moments $\mu_0, \mu_1, \ldots, \mu_{n+1}$. The idea is to replace μ_{n+1} by $\tilde{\mu}_{n+1}$ giving rise to a new measure $\tilde{\mu}$ such that

$$\left\langle Q_{n+2}, z^j \right\rangle_{\tilde{\mu}} = 0, \quad j = 1, 2, \ldots, n+1. \tag{4.5}$$

Assume that this measure $\tilde{\mu}$ exists and let $\{\tilde{\rho}_j\}_0^\infty$ be the corresponding sequence of monic Szegő polynomials.

From Theorem 2.1 we know that any polynomial of the form

$$Q_{n+2}(z) = c_n[z\tilde{\rho}_{n+1}(z) + \tau\tilde{\rho}^*_{n+1}(z)], \quad c_n \neq 0, |\tau| = 1 \tag{4.6}$$

satisfies (4.5) and by Theorem 2.2, that its zeros $z_1, \ldots, z_{n+1}$ are distinct and lie on $\mathbb{T}$. Furthermore, there exist positive coefficients $\tilde{\lambda}_1, \ldots, \tilde{\lambda}_{n+1}$ such that

$$I_{n+2}(f) = \sum_{j=1}^{n+1} \tilde{\lambda}_j f(z_j) = I_{\tilde{\mu}}(f), \quad \forall f \in \Lambda_{-(n+1),n+1}$$

i.e. $I_{n+2}(z^k) = I_{\tilde{\mu}}(z^k) = \tilde{\mu}_{-k}$, $k = 0, \pm 1, \ldots, \pm(n+1)$. Since $\tilde{\mu}_k = \mu_k$, $k = 0, \pm 1, \ldots, \pm n$, it follows that

$$I_{n+2}(f) = I_\mu(f), \quad \forall f \in \Lambda_{-n,n}.$$

Thus, the problem reduces to determining complex numbers $\tau \in \mathbb{T}$ and $\tilde{\mu}_{n+1}$ such that

(1) The linear functional $\tilde{\mu} : \Lambda_{-(n+1),n+1} \to \mathbb{C}$: $\tilde{\mu}(z^j) = \tilde{\mu}_j$, $j = 0, \pm 1, \ldots, \pm(n+1)$ with $\tilde{\mu}_j = \mu_j$, $j = 0, \ldots, n$, and $\tilde{\mu}_{-j} = \overline{\tilde{\mu}_{-j}}$, is positive definite.
(2) $Q_{n+2}(x_1) = Q_{n+2}(x_2) = 0$ with Q_{n+2} given by (4.6).

Making use of the Levinson algorithm, we can compute the monic polynomials $\rho_0, \ldots, \rho_n$ and $\tilde{\rho}_{n+1}$ from the moments $\mu_0, \ldots, \mu_n, \tilde{\mu}_{n+1}$ by the recurrence formulas

$$\left.\begin{aligned} \rho_{j+1}(z) &= z\rho_j(z) + \delta_{j+1}\rho_j^*(z) \\ \rho_{j+1}^*(z) &= \bar{\delta}_{j+1} z\rho_j(z) + \rho_j^*(z) \end{aligned}\right\}, \quad j = 0, \ldots, n-1 \tag{4.7}$$

ending with

$$\rho_n(z) = z\rho_{n-1}(z) + \delta_n \rho^*_{n-1}(z) \quad \text{and} \quad \tilde{\rho}_{n+1}(z) = z\rho_n(z) + \tilde{\delta}_{n+1}\rho^*_n(z). \tag{4.8}$$

Here $\tilde{\delta}_{n+1}$ represents the $(n+1)$th Schur parameter for $\tilde{\mu}$.

Finally, taking into account that finding $\tilde{\mu}_{n+1}$ such that $\tilde{\mu}$ is positive definite is equivalent to finding $\tilde{\delta}_{n+1}$ such that $|\tilde{\delta}_{n+1}| < 1$ (see e.g. [1]), our problem can be reformulated in the following terms.

Problem 4.3. Given the measure μ with monic Szegő polynomials $\{\rho_k\}_{k=0}^n$ and Schur parameters $\delta_k = \rho_k(0)$. Given also the numbers x_1 and x_2 on $\mathbb{T}$ with $x_1 \neq x_2$, find complex numbers $\tau \in \mathbb{T}$ and $\tilde{\delta}_{n+1} \in \mathbb{D}$ such that the polynomial Q_{n+2} defined by

$$Q_{n+2}(z) := z\tilde{\rho}_{n+1}(z) + \tau\tilde{\rho}^*_{n+1}(z), \quad \text{with } \tilde{\rho}_{n+1}(z) := z\rho_n(z) + \tilde{\delta}_{n+1}\rho^*_n(z) \tag{4.9}$$

vanishes at $z = x_1$ and $z = x_2$.

Thus we have come to the same problem recently solved by Jagels and Reichel in [2], although it is introduced in a different way.

5. Error estimates and convergence

In this section we shall be first concerned with the error estimates for the Szegő–Lobatto quadrature rules. Thus, fixing $n \in \mathbb{N}$ and given two distinct points x_1 and x_2 on $\mathbb{T}$, we will try to estimate the error corresponding of a Szegő–Lobatto quadrature, that is

$$R_{n+2}(f) := I_\mu(f) - I_{n+2}(f) = \int_{-\pi}^{\pi} f(e^{i\theta})d\mu(\theta) - \left[A_1 f(x_1) + A_2 f(x_2) + \sum_{j=1}^{n} \lambda_j f(z_j)\right] \tag{5.1}$$

with the nodes $\{z_j\}_{j=1}^n$ and weights A_1, A_2 and $\{\lambda_j\}_{j=1}^n$ as given in the previous section.

For this purpose, we first analyse the measure $\tilde{\mu}$ appearing in the construction of the Szegő–Lobatto rule. It is a new measure $\tilde{\mu}^{(n)}$ such that

$$I_\mu(L) = I_{\tilde{\mu}^{(n)}}(L) = I_{n+1}(L), \quad \forall L \in \Lambda_{-n,n}.$$

Let us see what happens as n tends to infinity. Therefore, suppose $f \in C(\mathbb{T})$, i.e., f is a continuous function on $\mathbb{T}$, and denote by $E_n(f)$ its minimax error in $\Lambda_{-n,n}$, that is

$$E_n(f) := \min\{\|f - T\|_{\mathbb{T}} : T \in \Lambda_{-n,n}\}. \tag{5.2}$$

As usual, $\|\cdot\|_A$ with A a compact set in $\mathbb{C}$, represents the uniform norm on A, i.e., $\|f\|_A = \max_{x\in A}|f(x)|$. Then the following holds.

Proposition 5.1. *Take $f \in C(\mathbb{T})$ and consider the measure $\tilde{\mu}^{(n)}$ as defined above. Then*

$$\left|I_\mu(f) - I_{\tilde{\mu}^{(n)}}(f)\right| \le 2\mu_0 E_n(f) \tag{5.3}$$

where $\mu_0 := I_\mu(1) = I_{\tilde{\mu}^{(n)}}(1)$.

Proof. Let $T_n \in \Lambda_{-n,n}$ be such that $\|f - T_n\|_{\mathbb{T}} = E_n(f)$. Then

$$|I_\mu(f) - I_{\tilde{\mu}^{(n)}}(f)| = |I_\mu(f) - I_\mu(T_n) + I_\mu(T_n) - I_{\tilde{\mu}^{(n)}}(f)| \le |I_\mu(f - T_n)| + |I_{\tilde{\mu}^{(n)}}(f - T_n)|$$

since $I_\mu(T_n) = I_{\tilde{\mu}^{(n)}}(T_n)$. Thus, the proof follows easily. □

Since it is known (see e.g. [10]) that $\lim_{n\to\infty} E_n(f) = 0$ one readily has the following consequence.

Corollary 5.2. *The sequence of measures $\{\tilde{\mu}^{(n)}\}_{n=1}^\infty$ converges weakly to the measure μ.*

After this, let us return to the estimation of the error $R_{n+2}(f)$. First assume that f is an analytic function on a domain G containing the unit circle and let $\Gamma = \partial G$ be its boundary. Let $F_\mu(z) := I_\mu((e^{i\theta} + z)/(e^{i\theta} - z))$ be the Herglotz–Riesz transform of the measure μ and write

$$F_{n+2}(z) := I_{n+2}\left(\frac{t+z}{t-z}\right) = A_1\left(\frac{x_1+z}{x_1-z}\right) + A_2\left(\frac{x_2+z}{x_2-z}\right) + \sum_{j=1}^{n}\lambda_j\left(\frac{z_j+z}{z_j-z}\right). \tag{5.4}$$

Then, from the Cauchy and Fubini theorems, it follows that

$$R_{n+2}(f) = \frac{1}{2\pi i}\int_\Gamma [F_\mu(z) - F_{n+2}(z)]\left(\frac{-f(z)}{2z}\right)dz \tag{5.5}$$

and accordingly

$$|R_{n+2}(f)| \le \frac{1}{4\pi}\ell(\Gamma)\|F_\mu - F_{n+2}\|_\Gamma \left\|\frac{f(z)}{z}\right\|_\Gamma \tag{5.6}$$

where $\ell(\Gamma)$ denotes the length of Γ. Thus, one sees that the error $|R_{n+2}(f)|$ is essentially controlled by the quantity $\|F_\mu - F_{n+2}\|_\Gamma$. In this respect, several computable upper bounds for $\|F_\mu - F_{n+2}\|_\Gamma$ were given in [11] when dealing with Szegő quadratures (see also [3] and [12] for particular cases). However these results cannot be used here, since in general $I_{n+2}(f)$ is not a Szegő rule for the measure μ. On the other hand, from Section 4, one knows that $I_{n+2}(f)$ is actually an $(n+2)$-point Szegő rule for the measure $\tilde{\mu}^{(n)}$. Set $\tilde{R}_{n+2}(f) := I_{\tilde{\mu}^{(n)}}(f) - I_{n+2}(f)$, then by (5.3) one readily has the following.

Proposition 5.3. *With the notation just introduced, one has*

$$|R_{n+2}(f)| \le 2\mu_0 E_n(f) + |\tilde{R}_{n+2}(f)|, \quad \text{with } f \in C(\mathbb{T}). \tag{5.7}$$

We can now make use of the results given in [11] along with (5.6)–(5.7) in order to estimate $|R_{n+2}(f)|$. Indeed, in [11] certain computable upper bounds are deduced and the sharper they are, the more difficult to compute them. For our purposes, we will take the simplest one so that the following holds [11].

Lemma 5.4. *Let μ be a positive measure on $\mathbb{T}$ and let $\{\rho_n(z)\}_0^\infty$ be its sequence of monic Szegő polynomials. Take $\tau \in \mathbb{T}$ and consider the corresponding n-point Szegő formula $I_n(f) = \sum_{j=1}^n \lambda_j f(z_j)$. Set $F_n(z) := \sum_{j=1}^n \lambda_j \frac{z_j+z}{z_j-z}$, then*

$$|F_\mu(z) - F_n(z)| \le \frac{8|z|^n}{(1-|z|^2)|1+\overline{\tau}\rho_n(z)/\rho_n^*(z)|}, \quad \forall z \in \mathbb{D} = \{z \in \mathbb{C} : |z| < 1\}. \tag{5.8}$$

When dealing with $z \in \mathbb{E} = \{z \in \mathbb{C} : |z| > 1\}$, it suffices to take into account that $F_\mu(z)$ and $F_n(z)$ satisfy $\overline{F_\mu(1/\overline{z})} = -F_\mu(z)$ and $\overline{F_n(1/\overline{z})} = -F_n(z)$, yielding

$$|F_\mu(z) - F_n(z)| \le \frac{8|z|^2}{|z|^n(|z|^2-1)|1+\tau\rho_n^*(z)/\rho_n(z)|}, \quad \forall z \in \mathbb{E}. \tag{5.9}$$

Given the prescribed nodes x_1 and x_2 on $\mathbb{T}$, define

$$a_j = \frac{x_j^{n-1}\overline{\rho_n(x_j)}}{\rho_n(x_j)} \in \mathbb{T}, \quad j = 1, 2. \tag{5.10}$$

Then from [2], if either $a_1x_1 = a_2x_2$ or $a_1 = a_2$, it is known that a Szegő formula can be constructed having x_1 and x_2 among its nodes. Thus, assume the generic case $a_1 \ne a_2$ and $a_1x_1 \ne a_2x_2$ and introduce the constants

$$c := -\frac{x_1 - x_2}{a_1x_1 - a_2x_2}, \qquad r := \left|\frac{a_1 - a_2}{a_1x_1 - a_2x_2}\right|. \tag{5.11}$$

Consider the circle C of center c and radius r, so that [2] $C \cap \mathbb{D} \ne \varnothing$. Take $\tilde{\delta}_{n+1} \in C \cap \mathbb{D}$ and set

$$\tau_n := -\frac{a_1x_1 - a_2x_2}{a_1 - a_2}\tilde{\delta}_{n+1} - \frac{x_1 - x_2}{a_1 - a_2} \in \mathbb{T}. \tag{5.12}$$

Under these conditions, there exists an $(n+2)$-point Szegő–Lobatto quadrature formula, $I_{n+2}(f) = A_1 f(x_1) + A_2 f(x_2) + \sum_{j=1}^n \lambda_j f(z_j)$ so that the nodes (including both x_1 and x_2) are the zeros of the polynomial

$$Q_{n+2}(z) = z\tilde{\rho}_{n+1}(z) + \tau_n\tilde{\rho}_{n+1}^*(z), \quad \text{with } \tilde{\rho}_{n+1}(z) = z\rho_n(z) + \tilde{\delta}_{n+1}\rho_n^*(z). \tag{5.13}$$

Here $\rho_n(z)$ denotes as usual the nth monic Szegő polynomial for the measure μ.

Remark 5.5. If $\delta_{n+1} \in C \cap \mathbb{D}$, then one can take $\tilde{\delta}_{n+1} = \delta_{n+1}$ and the above $(n+2)$-point Szegő–Lobatto quadrature formula is actually an $(n+2)$-point Szegő formula and the upper bounds valid for Szegő formulas can be used. Thus assume also that $\delta_{n+1} \notin C \cap \mathbb{D}$.

We are now in a position to state the following theorem.

Theorem 5.6. *Assume as above that C is the circle with center $c \ne \infty$ and radius $r \ne 0$, given by (5.11), and the Schur parameter δ_{n+1} satisfies $\delta_{n+1} \notin C \cap \mathbb{D} \ne \varnothing$. Moreover τ_n is given by (5.12) and $\tilde{\rho}_{n+1}$ by (5.13). Let f be an analytic function on a domain $G \supset \mathbb{T}$ with boundary $\Gamma = \partial G$. Set*

$$K_1^{(n)} := \left\|\frac{|z|^{n+2}}{(1-|z|^2)|1+\overline{\tau}_n z\tilde{\rho}_{n+1}(z)/\tilde{\rho}_{n+1}^*(z)|}\right\|_{\Gamma\cap\mathbb{D}},$$

$$K_2^{(n)} := \left\|\frac{|z|^{-n}}{(|z|^2-1)|1+\tau_n\tilde{\rho}_{n+1}(z)/(z\tilde{\rho}_{n+1}^*(z))|}\right\|_{\Gamma\cap\mathbb{E}},$$

and $K_n := \max\{K_1^{(n)}, K_2^{(n)}\}$*. Then the approximation error* $R_{n+2}(f) := I_\mu(f) - I_{n+2}(f)$ *for the the Szegő–Lobatto quadrature satisfies*

$$|R_{n+2}(f)| \leq 2\left[\frac{\ell(\Gamma)}{\pi}K_n\|f(z)/z\|_\Gamma + \mu_0 E_n(f)\right] \tag{5.14}$$

where $\ell(\Gamma)$ *denotes the length of* Γ *and* $E_n(f)$ *the minimax error of* f *in* $\Lambda_{-n,n}$.

As an alternative to the upper bound (5.14) we can also give a more generic bound deduced from the recent paper [13]. Indeed from [13, Theorem 1], it holds that the following is true.

Theorem 5.7. *Under the same assumptions as in Theorem 5.6, there exist positive numbers* r *and* R *such that* $r < 1 < R$ *and so that*

$$|R_{n+2}(f)| \leq 2\mu_0\|f\|_{\gamma_r\cup\gamma_R}\left(\frac{r^{n+1}}{1-r^2} + \frac{R^{1-n}}{R^2-1}\right) \tag{5.15}$$

where for $\alpha > 0$, γ_α *denotes the circle with radius* α *centered at the origin.*

Remark 5.8. Theorem 1 in [13] was proved in a more general framework involving quadrature rules exactly integrating certain rational functions with prescribed poles not on $\mathbb{T}$. When all the poles collapse at the origin and infinity, the rational functions become Laurent polynomials. The upper bound given in [13] is rather universal and essentially depending on the domain of analyticity of f and the domain of validity of the quadrature rule. In our case, this domain is $\Lambda_{-n,n}$.

In the rest of the section we will deal with some aspects related to convergence. For $n > 2$, we take two distinct points on $\mathbb{T}$ depending on n, namely $x_1^{(n)}$ and $x_2^{(n)}$ and consider an n-point Szegő–Lobatto quadrature rule as previously defined for μ, that is

$$I_n(f) = A_1^{(n)}f(x_1^{(n)}) + A_2^{(n)}f(x_2^{(n)}) + \sum_{j=1}^{n-2}\lambda_j^{(n)}f(z_j^{(n)}) = I_\mu(f), \qquad \forall f \in \Lambda_{-(n-2),(n-2)}. \tag{5.16}$$

Since the weights in (5.16) are positive and recalling that the sequence of minimax values $E_n(f)$ tends to zero, we can easily prove, using standard arguments that the following holds.

Theorem 5.9. *Let* $\{I_n(f)\}_{n>2}$ *be a sequence of Szegő–Lobatto quadrature rules for a measure* μ*. Then* $\lim_{n\to\infty} I_n(f) = I_\mu(f)$ *for any bounded function* f *integrable with respect to* μ *on* $\mathbb{T}$.

We are now interested in the estimation of the rate of convergence. That is in estimating $\limsup_{n\to\infty}|R_n(f)|^{1/n}$ where $R_n(f)$ denotes the error for the nth rule, i.e., $R_n(f) = I_\mu(f) - I_n(f)$. Thus from (5.6) one can write

$$|R_n(f)| \leq M(f)\|F_\mu - F_n\|_\Gamma \tag{5.17}$$

with $M = M(f)$ a constant depending on f but independent of n and where we are assuming that $f(z)$ is analytic in a region $G \supset \mathbb{T}$, Γ being its boundary. As usual $F_\mu(z)$ and F_n denote Herglotz–Riesz transforms, i.e.,

$$F_\mu(z) := I_\mu\left(\frac{t+z}{t-z}\right) \quad \text{and} \quad F_n(z) := I_n\left(\frac{t+z}{t-z}\right), \qquad t = e^{i\theta}.$$

From (5.17) one sees that $\limsup_{n\to\infty}|R_n(f)|^{1/n} \leq \limsup_{n\to\infty}\|F_\mu - F_n\|_\Gamma^{1/n}$ and consequently one needs to compute $\|F_\mu - F_n\|_\Gamma$. By Corollary 4.1, $I_n(f)$ is exact in $\Lambda_{-p,q}$, where p and q are integers such that $0 \leq p, q \leq n-2$ and $p+q = n-1$. Thus from [14] one readily gets

$$H_n(z) := F_\mu(z) - F_n(z) = \frac{2z^{p+1}}{Q_n(z)}\int_{-\pi}^{\pi}\frac{e^{-ip\theta}Q_n(e^{i\theta})}{e^{i\theta}-z}d\mu(\theta), \qquad \forall z \notin \mathbb{T}. \tag{5.18}$$

If we take $p = n-2$, (i.e., $q = 1$), then

$$H_n(z) = \frac{2z^{n-1}}{Q_n(z)}\int_{-\pi}^{\pi}\frac{x^{-(n-2)}Q_n(x)}{x-z}d\mu(\theta), \qquad x = e^{i\theta}. \tag{5.19}$$

Here $Q_n(z)$ is the nodal polynomial associated with $I_n(f)$, i.e., $Q_n(z) = c_n(z - x_1^{(n)})(z - x_2^{(n)})\prod_{j=1}^{n-2}(z - z_j^{(n)})$, $c_n \neq 0$. From (5.18) or (5.19) we see that in order to compute $|H_n(z)|^{1/n}$ we need to study the behaviour of $|Q_n(z)|^{1/n}$ for $z \notin \mathbb{T}$ and $\|Q_n\|_{\mathbb{T}}^{1/n}$.

From Section 4 it is deduced that for each n, $Q_n(z)$ is a polynomial of degree n, para-orthogonal with respect to a measure $\tilde{\mu}^{(n)}$. For each $n = 3, 4, \ldots$ let us denote by $\{\varphi_{k,n}\}_{k=0}^{\infty}$ the sequence of orthogonal Szegő polynomials for the measure $\tilde{\mu}^{(n)}$, so that we can write $Q_n(z) = \varphi_{n,n}(z) + \tau_n\varphi_{n,n}^*(z)$, $\tau_n \in \mathbb{T}$, $n > 2$. Now making use of the results given in [15,16], and proceeding as in [17], we deduce the following result.

Lemma 5.10. *With the previous notation, it holds that*

(1) $\lim_{n\to\infty}|Q_n(z)|^{1/n} = |z|$*, uniformly on compact subsets of* $\mathbb{E}$

Table 1
Center and radius of the circles defined in (5.11) for the Rogers–Szegő polynomials with fixed nodes $x_1 = e^{i\pi/12}$ and $x_2 = e^{-i\pi/20}$, $q = 0.5$ and $n = 6, 10, 14$ and 20.

Nodes n	Radius r	Center c
6	0.977	$0.185 + 0.095i$
10	0.701	$0.267 + 0.222i$
14	1.971	$-0.636 - 0.790i$
20	1.001	$-0.075 - 0.195i$

(2) $\lim_{n\to\infty} |Q_n(z)|^{1/n} = 1$, *uniformly on compact subsets of* $\mathbb{D}$
(3) $\lim_{n\to\infty} M_n^{1/n} = 1$ *where* $M_n = \|Q_n\|_{\mathbb{T}} = \max_{x\in\mathbb{T}} |Q_n(x)|$.

Thus by Lemma 5.10, (5.17), (5.19), and the fact that $\overline{H_n(1/\bar{z})} = -H_n(z)$, we can prove:

Theorem 5.11. *Let* $\{I_n(f)\}_{n=3}^{\infty}$ *be a sequence of Szegő–Lobatto rules and let* f *be an analytic function in a domain* $G \supset \mathbb{T}$, *with boundary* Γ. *Set* $R_n(f) = I_\mu(f) - I_n(f)$. *Then*

$$\limsup_{n\to\infty} |R_n(f)|^{1/n} \le r < 1, \quad r = \max\{r_1, r_2\}$$

where $r_1 := \max\{|z| : z \in \Gamma \cap \mathbb{D}\}$ *and* $r_2 := \max\{1/|z| : z \in \Gamma \cap \mathbb{E}\}$.

Remark 5.12. If we compare the estimates of the rate of convergence for a sequence of Szegő–Lobatto formulas as given in Theorem 5.11 with the estimates of the rates of convergence for a sequence of Szegő rules (see e.g. [14]), then we see that both coincide. Thus, as might be expected, fixing two nodes, does not affect the rate of convergence.

6. Numerical examples

Let us consider the absolutely continuous measure on $[-\pi, \pi]\mathrm{d}\mu(\theta) = \omega(\theta)\mathrm{d}\theta$, where $\omega(\theta)$ is given by:

$$\omega(\theta) := \frac{1}{\sqrt{2\pi \log\left(\frac{1}{q}\right)}} \sum_{j=-\infty}^{\infty} \exp\left(\frac{-(\theta - 2\pi j)^2}{2\pi \log\left(\frac{1}{q}\right)}\right), \quad q \in (0, 1).$$

This weight gives rise to the known family of Roger–Szegő polynomials.

An explicit expression for the corresponding monic polynomial is known (see [7]):

$$\rho_n(z) = \begin{cases} \displaystyle\sum_{j=0}^{2k} (-1)^j \begin{bmatrix} 2k \\ j \end{bmatrix}_q q^{\frac{2k-j}{2}} z^j, & n = 2k, \\ \displaystyle\sum_{j=0}^{2k+1} (-1)^j \begin{bmatrix} 2k+1 \\ 2k+1-j \end{bmatrix}_q q^{\frac{j}{2}} z^j, & n = 2k+1, \end{cases} \tag{6.1}$$

where

$$\begin{bmatrix} n \\ j \end{bmatrix}_q := \frac{(1-q^{n-j+1})(1-q^{n-j+2})\dots(1-q^n)}{(1-q)(1-q^2)\dots(1-q^j)}.$$

Moreover, a simple explicit formula for the moments in terms of the parameter q is also known (see [7] and also, [18]).

$$\mu_k := \int_{-\pi}^{\pi} e^{-ik\theta}\omega(\theta)\mathrm{d}\theta = q^{\frac{k^2}{2}}, \quad k \in \mathbb{Z}. \tag{6.2}$$

Let us fix the parameter q as $q = 0.5$, several values of the degree of the polynomial, say $n = 6, 10, 14, 20$ and the two fixed points on $\mathbb{T}$ as $x_1 = e^{i\pi/12}$, and $x_2 = e^{-i\pi/20}$.

In this case, since both inequalities $a_1 \ne a_2$ and $a_1x_1 \ne a_2x_2$, hold for $\{a_j\}_{j=1}^2$ given by (5.10), it follows by [2] that we are in the generic case. Consider the circle C of center c and radius r, so that $C \cap \mathbb{D} \ne \varnothing$ (see [2]). Then, the center c and radius r in (5.11) are approximately given in Table 1.

We have drawn each circumference along with the unit circle. You can see it in Fig. 1.

According to Fig. 1, in each case, we have chosen the parameters $\tilde{\delta}_{n+1} \in C \cap \mathbb{D}$ and calculated, by formula (5.12), the parameters $\tau \in \mathbb{T}$. The approximate results are displayed in Table 2.

Under these conditions, there exists an $(n+2)$-point Szegő–Lobatto quadrature formula,

$$I_{n+2}(f) = A_1 f(x_1) + A_2 f(x_2) + \sum_{j=1}^{n} \lambda_j f(z_j),$$

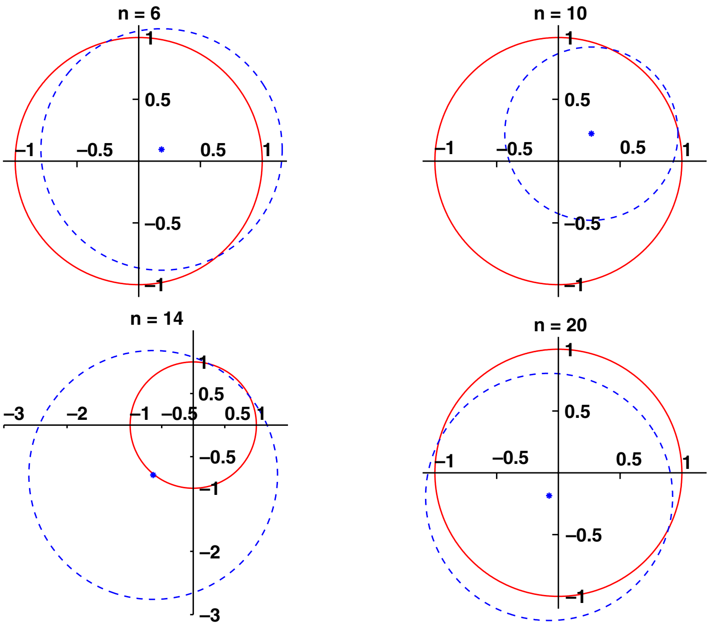


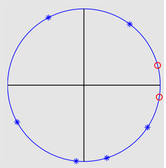
Fig. 1. The circles $C(c, r)$ corresponding to the data of Table 1 are plotted in dashed lines, the unit circle in solid line.

Table 2
With the data of Table 1, the chosen parameter $\tilde{\delta}_{n+1} \in C \cap \mathbb{D}$, and the corresponding $\tau \in \mathbb{T}$ given by (5.12) are listed.

Nodes n	$\tilde{\delta}_{n+1}$	τ
6	$-0.864\mathrm{i}$	$0.137 + 0.991\mathrm{i}$
10	$0.869\mathrm{i}$	$0.429 - 0.903\mathrm{i}$
14	$0.500 + 0.820\mathrm{i}$	$-0.533 - 0.846\mathrm{i}$
20	$0.803\mathrm{i}$	$-0.023 - 1.000\mathrm{i}$

Table 3
The nodes and weights of Szegő–Lobatto formula with $n = 6$ free nodes and the two fixed nodes $x_1 = \mathrm{e}^{\mathrm{i}\pi/12}$ and $x_2 = \mathrm{e}^{-\mathrm{i}\pi/20}$ considered before. The nodes are plotted in the figure on the right. The prefixed nodes are indicated by circles, the other by stars.

Nodes	Arg. nodes	Weights
−0.875+0.484i	3.647e+00	0.475682e−02
−0.465−0.885i	2.055e+00	0.199333e−01
−0.101+0.995i	4.612e+00	0.509562e−01
0.300−0.954i	−1.266e+00	0.110050e+00
0.601+0.799i	9.262e−01	0.182012e+00
0.833−0.556i	−5.854e−01	0.228866e+00
0.966+0.259i	**2.618e−01**	0.273795e+00
0.988−0.156i	**−1.571e−01**	0.129630e+00



so that the nodes (including both x_1 and x_2) are the zeros of the polynomial

$$Q_{n+2}(z) = z\tilde{\rho}_{n+1}(z) + \tau_n\tilde{\rho}^*_{n+1}(z), \quad \text{with } \tilde{\rho}_{n+1}(z) = z\rho_n(z) + \tilde{\delta}_{n+1}\rho^*_n(z),$$

where $\rho_n(z)$ denotes the monic Roger–Szegő polynomial given by (6.1).

We have computed the nodes and weights for the corresponding Szegő–Lobatto quadrature formula for $n = 6$. The results are given in Table 3.

Note that the fixed points on the unit circle:

$$x_1 = \mathrm{e}^{\mathrm{i}\pi/12} \approx 0.9659258262795216 + 0.2588190450910\,53\mathrm{i}$$

and

$$x_2 = \mathrm{e}^{-\mathrm{i}\pi/20} \approx 0.98768834059171\,22 - 0.15643446504697572\mathrm{i},$$

are now recovered as nodes in the quadrature formula.

As for the weights $\{\lambda_j\}_{j=1}^{n+2}$, which are all positive, they were calculated as follows. Since (see [19])

$$\lambda_j = \frac{1}{2\mathrm{Re}\{z_j\overline{\varphi^*_{n+1}(z_j)}\varphi^{*'}_{n+1}(z_j)\} - n|\varphi^*_{n+1}(z_j)|^2}, \quad j = 1, \ldots, n+2,$$

Table 4
The absolute errors and the error bounds for Szegő–Lobatto quadrature formulas applied to function f_1.

n	Absolute error	Error bound. ($r = 0.57$)
6	8.0136×10^{-3}	4.89949×10^{-1}
10	5.6092×10^{-4}	5.17190×10^{-2}
14	4.1999×10^{-5}	5.45946×10^{-3}
20	3.7410×10^{-7}	1.87240×10^{-4}

Table 5
The absolute errors and the error bounds for Szegő–Lobatto quadrature formulas applied to function f_2.

n	Absolute error	Error bound. ($r = 0.2, R = 1.8$)
6	3.33902×10^{-3}	6.96045×10^{-1}
10	2.33717×10^{-4}	6.62686×10^{-2}
14	1.74994×10^{-5}	6.31266×10^{-3}
20	1.55855×10^{-7}	1.85599×10^{-4}

Table 6
The absolute errors and the error bounds for Szegő–Lobatto quadrature formulas applied to function f_3.

n	Absolute error	Error bound. ($R = 7$)
6	6.79314×10^{-5}	2.71869×10^{-3}
10	7.49269×10^{-9}	1.11323×10^{-6}

where $\varphi^*_{n+1}(z) = c\rho^*_{n+1}(z)$, we can write $\lambda_j^{-1} = |c|^2 \lambda_j^{*-1}$, with

$$\lambda_j^* = \frac{1}{2\mathrm{Re}\{z_j \overline{\rho^*_{n+1}(z_j)}\rho^{*'}_{n+1}(z_j)\} - n|\rho^*_{n+1}(z_j)|^2}, \quad j = 1, \dots, n+2.$$

Therefore, it remains to determine the constant $|c|^2$. But, since the quadrature formula is exact for $f \equiv 1$, and $\mu_0 = 1$ (see (6.2)), it follows that $|c|^2 = \sum_{j=1}^{n+2} \lambda_j^*$.

Now, we have computed the Szegö–Lobatto quadrature formulas for the following three different choices of functions:

$$f_1(z) = \frac{z^2 - 1}{2iz(z - 0.5)}, \qquad f_2(z) = \frac{z^2 + 1}{2z(z - 2)}, \qquad f_3(z) = e^z.$$

Note that f_1 is analytic in $G_1 = \{z : |z| \geq r\} \supsetneqq \mathbb{T}$, where $1 > r > \frac{1}{2}$. The function f_2 is analytic in $G_2 = \{z : r \leq |z| \leq R\} \supsetneqq \mathbb{T}$, where $0 < r < 1 < R < 2$. And for f_3 in $G_3 = \{z : |z| \leq R\} \supsetneqq \mathbb{T}$, for all $R > 1$.

The results are displayed in the following Tables 4–6. We have also included the upper bound given in formula (5.15). For this purpose, we have considered the functions analytic in the domains above described for particular choices of r and R.

The exact integral was calculated using the following equality, (see [18]) which allows us to pass from the unit circle to an easily computable real integral:

$$\int_{-\pi}^{\pi} f(\theta)\omega(\theta)\mathrm{d}\theta = \int_{-\infty}^{\infty} f(x)\gamma(x)\mathrm{d}x,$$

where $\omega(\theta)$ is the Roger–Szegö weight function and $\gamma(x) = (1/\sqrt{2\pi \log 1/q})\mathrm{e}^{\frac{-x^2}{2\pi \log 1/q}}$.

Note that the upper bounds are rough over-estimations of the error.

Remark 6.1. For the above computations we used the program Mathematica, which uses in its computation, 10 decimal digits. Therefore, we got the exact result indeed up to machine precision for the functions f_1 and f_2. Also, for the function f_3, since with $n = 10$ we achieved the machine precision, we omitted the results for $n = 14$ and $n = 20$, which are similar to the error given by $n = 10$.

Acknowledgment

We thank the anonymous referees for their detailed and constructive comments that helped us to provide a much better paper.

This work is partially supported by the Direción General de Investigación, Ministerio de Educación y Ciencia, under grant MTM2005-08571. The work of the first author is partially supported by the Fund for Scientific Research (FWO), projects "RAM: Rational modelling: optimal conditioning and stable algorithms", grant #G.0423.05 and the Belgian Programme on Interuniversity Poles of Attraction, initiated by the Belgian State, Prime Minister's Office for Science, Technology and Culture. The scientific responsibility rests with the author.

References

[1] W.B. Jones, O. Njåstad, W.J. Thron, Moment theory, orthogonal polynomials, quadrature and continued fractions associated with the unit circle, Bull. London Math. Soc. 21 (1989) 113–152.
[2] C. Jagels, L. Reichel, Szegő-Lobatto quadrature rules, J. Comput. Appl. Math. 200 (1) (2007) 116–126.
[3] L. Daruis, P. González-Vera, Szegő polynomials and quadrature formulas on the unit circle, Appl. Numer. Math. 36 (1) (2000) 79–112.
[4] A. Bultheel, P. González-Vera, E. Hendriksen, O. Njåstad, Orthogonality and quadrature on the unit circle, in: C. Brezinski, L. Gori, A. Ronveaux (Eds.), Orthogonal Polynomials and their Applications, in: IMACS Annals on Computing and Applied Mathematics, vol. 9, J.C. Baltzer AG, Basel, 1991, pp. 205–210.
[5] W.B. Gragg, Positive definite Toeplitz matrices, the Arnoldi process for isometric operators, and Gaussian quadrature on the unit circle, J. Comput. Appl. Math. 46 (1993) 183–198.
[6] M.J. Cantero, L. Moral, L. Velázquez, Measures and para-orthogonal polynomials on the unit circle, East J. Approx. 8 (2002) 447–464.
[7] B. Simon, Orthogonal polynomials on the unit circle. Part 1: Classical Theory, in: Colloquium Publications, vol. 54, AMS, 2005.
[8] M.J. Cantero, R. Cruz-Barroso, P. González-Vera, A matrix approach to the computation of quadrature formulas on the interval, Appl. Numer. Math. 58 (3) (2008) 296–318.
[9] E. Godoy, F. Marcellan, Orthogonal polynomials and rational modification of measures, Canad. J. Math. 45 (1993) 930–943.
[10] L. Daruis, P. González-Vera, Some results about interpolation with nodes on the unit circle, Indian J. Pure Appl. Math. 31 (10) (2000) 1273–1296.
[11] W.B. Jones, H. Waadeland, Bounds for remainder terms in Szegő quadrature on the unit circle, in: Approximation and Computation, in: Internat. Ser. of Numer. Math., vol. 119, Birkhäuser Verlag, 1995, pp. 325–342. (A Festschrift in honor of Walter Gautschi).
[12] L. Daruis, P. González-Vera, O. Njåstad, Szegő quadrature formulas for certain Jacobi-type weight functions, Math. Comp. 71 (238) (2002) 683–701.
[13] B. de la Calle Ysern, P. González-Vera, Rational quadrature formulas on the unit circle with arbitrary poles, Numer. Math. 107 (4) (2007) 559–587.
[14] P. González-Vera, J.C. Santos-León, O. Njåstad, Some results about numerical quadrature on the unit circle, Adv. Comput. Math. 5 (1996) 297–328.
[15] G. López-Lagomasino, On the asymptotics of the ratio of orthogonal polynomials and convergence of multipoint Padé approximants, Math. USSR-Sb. 56 (1987) 207–219.
[16] G. López-Lagomasino, Asymptotics of polynomials orthogonal with respect to varying measures, Constr. Approx. 5 (1989) 199–219.
[17] A. Bultheel, P. González-Vera, E. Hendriksen, O. Njåstad, On the convergence of multipoint Padé-type approximants and quadrature formulas associated with the unit circle, Numer. Algorithms 13 (1996) 321–344.
[18] R. Cruz-Barroso, P. González-Vera, F. Perdomo-Pío, Quadrature formulas associated with Rogers–Szegő polynomials, Comput. Math. Appl. 57 (2) (2009) 308–323.
[19] A. Bultheel, R. Cruz-Barroso, K. Deckers, P. González-Vera, Rational Szegő quadratures associated with Chebyshev weight functions, Math. Comp. 78 (2009) 1031–1059. (Published online December 9, 2008).